

Motion of wave packets in regular and chaotic systems

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The quantum energy spectrum of a system which is classically integrable consists of families of nearly equidistant levels. There is no such regularity for a classically chaotic system. As a consequence, a small wave packet, initially centered in a regular region of phase space, will slowly disperse while following the (almost) periodic classical trajectory. A wave packet placed in a chaotic region will disperse much more rapidly. These predictions are illustrated by calculating the evolution of two wave packets with the *same* mean energy in the Hénon-Heiles model.

I. INTRODUCTION

Classical Hamiltonian systems with N degrees of freedom have two essentially different types of orbits.^{1,2} "Regular" orbits, such as those of integrable systems, are multiply periodic in time. They lie on N -dimensional tori in phase space and neighboring orbits separate at a rate which is roughly linear in time. On the other hand, "irregular" or "chaotic" orbits explore higher dimensional domains of phase space (possibly the entire energy hypersurface) and neighboring orbits separate exponentially. A small cluster of points thus spreads in a finite time so as to come arbitrarily close to *any* point of the accessible phase space. This "mixing" behavior is usually construed as the rationale for irreversibility in statistical physics.³

There has been considerable controversy whether a similar dichotomy exists in quantum theory. There is no quantum equivalent to classical "neighboring orbits." If we follow the evolution of neighboring quantum states ϕ and $\phi + \delta\phi$, their scalar product $(\phi, \phi + \delta\phi)$ is constant in time. Many authors⁴⁻¹⁰ attempted to find a qualitatively different behavior of the "survival" probability

$$P(t) = |(\phi, \exp(-iHt/\hbar)\phi)|^2 \quad (1)$$

of an initial state ϕ , and obtained conflicting results. It seems to us that $P(t)$ cannot be a reliable criterion to distinguish regular from chaotic states. Intuitively, a quickly decaying $P(t)$ should be the hallmark of a chaotic system. However, a set of *uncoupled* harmonic oscillators, with *incommensurate* periods, also has a quickly decaying $P(t)$, although it is trivially integrable. (Strictly speaking, this system is almost periodic, but the time for a recurrence may be inordinately long.¹¹)

In Sec. II of this paper, we show that there is marked difference in the *rate of spreading of wave packets* moving in the regular vs chaotic regions of phase space. This result ought to be expected. As shown long ago by Madelung,¹² if we write the wave function as

$$\psi = \sqrt{\rho} e^{iS/\hbar} \quad (2)$$

with real ρ and S , then the real and imaginary parts of the time-dependent Schrödinger equation for a particle of mass m in a potential V are

$$\frac{\partial \rho}{\partial t} + \nabla \cdot \left(\rho \frac{\nabla S}{m} \right) = 0 \quad (3)$$

and

$$-\frac{\partial S}{\partial t} = \frac{1}{2m} (\nabla S)^2 + V - \frac{\hbar^2}{2m} \frac{\nabla^2 \sqrt{\rho}}{\sqrt{\rho}}. \quad (4)$$

Equation (3) shows that the probability density ρ flows as a classical fluid with velocity $\nabla S/m$. Equation (4), apart from the last term (of order \hbar^2) is the classical Hamilton-Jacobi equation¹³ for a particle of mass m in a potential V . Therefore, as long as we can neglect that last term, we expect a quantum wave packet to spread at the same rate as a classical Gibbs ensemble of particles in the same potential. (However, this analogy must ultimately break down, as shown below.)

In Sec. III, we explain these different rates of spreading of wave packets by qualitatively different structures of the energy spectra. A system which is classically integrable has families of nearly equidistant energy levels. There is no such regularity for the quantum energy spectrum of a system which is classically chaotic.

Finally, Sec. IV discusses some limitations of the correspondence principle. In particular, it is shown that there is no "area preserving" theorem in quantum mechanics. Some open problems are briefly mentioned in Sec. V.

II. WAVE PACKETS ON PERIODIC ORBITS

This section describes a numerical experiment in which we followed the evolution of wave packets initially given as

$$\psi_0(x, y) = (\pi\hbar)^{-1/2} \exp \left[-\frac{x^2}{2\hbar} + \frac{ix_0 x}{\hbar} - \frac{(y - y_0)^2}{2\hbar} \right], \quad (5)$$

where \dot{x}_0 and y_0 are constants, to be defined below. The Hamiltonian was taken as that of the Hénon-Heiles model¹⁴

$$H = \frac{1}{2}(\dot{p}_x^2 + \dot{p}_y^2 + x^2 + y^2) + x^2 y - \frac{1}{3}y^3. \quad (6)$$

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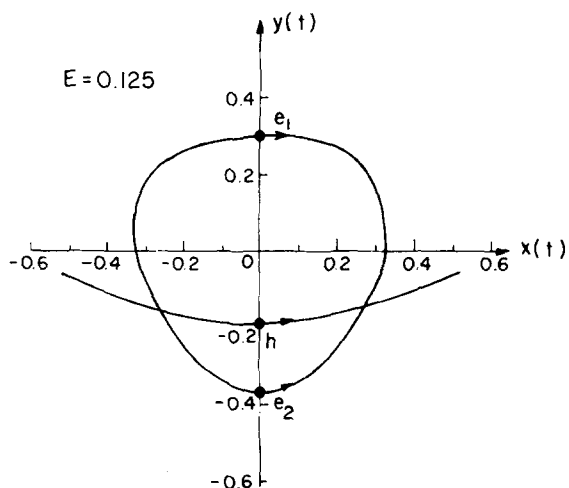


FIG. 1. Some periodic orbits of the Hénon-Heiles system (see Table I for details).

We compared wave packets initially centered on three classical *periodic* orbits, all at the *same* energy $E = 0.125$. These orbits are shown on Fig. 1 and their initial parameters¹⁵ are listed in Table I.

We considered several values of \hbar , the smallest one being $\hbar = 0.015$ (because of computer limitations). With that value of \hbar , we took 324 basis functions (products of oscillator eigenfunctions in the x and y directions) and diagonalized the truncated Hamiltonian matrix. Because of this truncation, the quantum system which we investigated is not a faithful analog of the classical Hénon-Heiles oscillator. It is a system with a finite number of energy levels, some of which lying above the classical dissociation limit $E_d = 0.1666$. The true Hénon-Heiles system would have only metastable levels, those above E_d having very short lifetimes. Nevertheless, we obtained good qualitative agreement with the classical motion, as shown below.

From the eigenvectors $u_n(x, y)$ we obtained the expansion coefficients of the various initial wave functions

$$C_n = \int \overline{u_n(x, y)} \psi_0(x, y) dx dy. \quad (7)$$

We thereafter obtained expectation values as usual.

The results are shown in Figs. 2 to 4, where we plotted the classical value of x together with a shaded area giving the "size" of the wave packet, namely,

TABLE I. The three periodic orbits. The other initial parameters are $x_0 = 0$, $y_0 = 0$, and $\dot{x}_0 > 0$ which is computed from the total energy $E = 0.125$ and Eq. (6). The labels e and h refer to "elliptic" and "hyperbolic" fixed points of the classical Poincaré map.

Orbit	Period	y_0
e_1 (stable)	6.08343	0.302666817
e_2 (stable)	6.08343	-0.372312784
h (unstable)	6.90853	-0.185405087

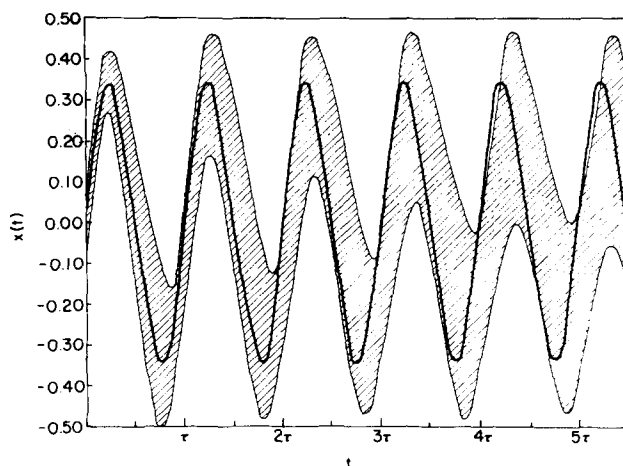


FIG. 2. Comparison of the classical periodic motion and of the evolution of a wave packet for a stable orbit. The solid line is the classical $x(t)$ and the hatched area represents $\langle x \rangle \pm \Delta x$ of the wave packet. Note that the classical and quantum periods are slightly different. This is due to the finite size of the wave packet which includes many classical trajectories with different periods.

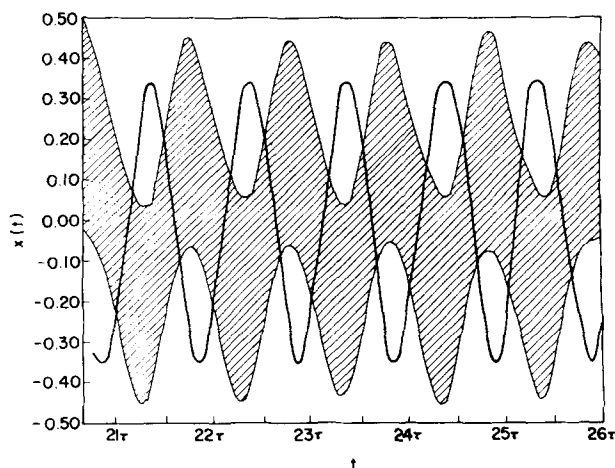


FIG. 3. Same as Fig. 2, but at a later time, to show the slow spreading of the wave packet.

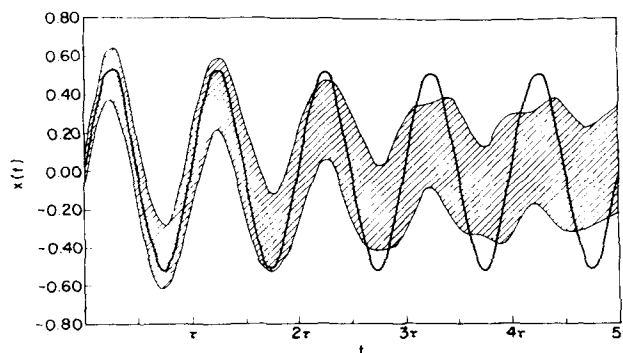


FIG. 4. Same as Fig. 2, but for an unstable orbit. The wave packet spreads very fast and then "settles" around the equilibrium value $\langle x \rangle = 0$.

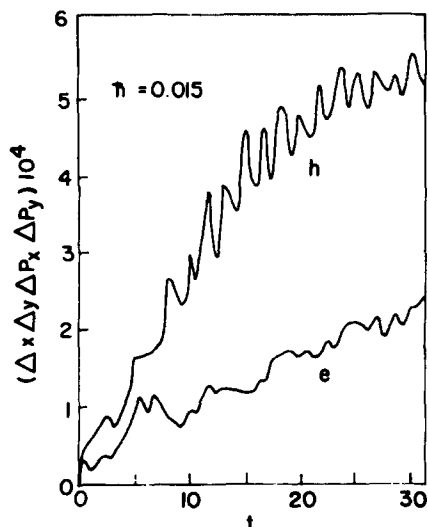


FIG. 5. The canonically invariant product $\Delta x \Delta p_x \Delta y \Delta p_y$, for both wave packets.

$$\langle x \rangle \pm \Delta x = \langle x \rangle \pm (\langle x^2 \rangle - \langle x \rangle^2)^{1/2}. \tag{8}$$

It is seen that the regular wave packet follows the classical orbit (with almost the same period) and slowly spreads around it, while the chaotic wave packet diffuses through the entire available phase space in a very short time.

In those figures we singled out x , one of the four canonical variables. Figure 5 shows the behavior of the canonically invariant product $\Delta x \Delta p_x \Delta y \Delta p_y$. There can be no doubt that wave packet initially centered on an unstable periodic orbit spreads much more rapidly than the one centered on a stable orbit.

III. ENERGY SPECTRA

These results are perhaps not surprising, in view of the classical analogy displayed by the Madelung equations, but they ought to be explained in terms of quantum theory alone. After all, we have the same Hamiltonian, therefore, the same energy spectrum, and wave packets of the same size, in particular, the same mean energy, only initially located at different positions. Why is there such a qualitative difference in their behavior?

The answer becomes apparent when we compute the populations $|C_i|^2$ of the various energy levels, as shown in Fig. 6. It is readily seen that the levels involved in the regular wave packet are nearly equidistant, so that its motion is indeed nearly periodic. On the other hand, as there is no regularity in the energy levels involved in the chaotic wave packet, the corresponding energy eigenfunctions are quickly dephased and the wave packet spreads through the entire domain covered by these wave functions.

In this connection, one may recall the different morphologies of the regular and irregular energy eigenfunctions.¹⁶ The regular states are associated with the classical tori in phase space and have intense anisotropic interference oscillations on the caustics of clas-

sical orbits. On the other hand, irregular states have anticaustics at the classical boundaries. One may therefore expect that in the semiclassical limit $\hbar \rightarrow 0$, as the various wave packets become very small compared to their mutual distance, they are not only almost orthogonal

$$S_{eh} \equiv |(\phi_e, \phi_h)|^2 = \left| \sum_n \bar{C}_{en} C_{hn} \right|^2 \approx 0, \tag{9}$$

but "superorthogonal"

$$\bar{S}_{eh} \equiv \left(\sum_n |C_{en} C_{hn}| \right)^2 \approx 0. \tag{10}$$

Here, ϕ_e and ϕ_h denote the initial states of the wave packets centered at the elliptic (stable) and hyperbolic (unstable) fixed points, respectively. In this connection, we may note that \bar{S}_{eh} is the largest value of the overlap of the two wave functions taken at any two times

$$\bar{S}_{eh} = \max \left| \sum_n \bar{C}_{en} C_{hn} \exp[iE_n(t_e - t_h)] \right|^2. \tag{11}$$

By suitably choosing t_e and t_h , this sum can be made arbitrarily close to $\sum |C_{en} C_{hn}|$. The physical meaning of superorthogonality is that *different energy levels are involved in the two wave functions*.

We have tested this prediction and the results are shown in Figs. 7 and 8. As we decrease \hbar , the chaotic wave packet tends to become more and more superorthogonal to the regular ones. On the other hand, the two regular wave packets tend to have $\bar{S} = 1$, which means that all their C_n have the same magnitude, only different phases. This is due to the fact that each one of the two classical orbits e_1 and e_2 is the mirror image of the other (see Fig. 1) and can be transformed into it by a time translation (half a period) followed by a time reflection.

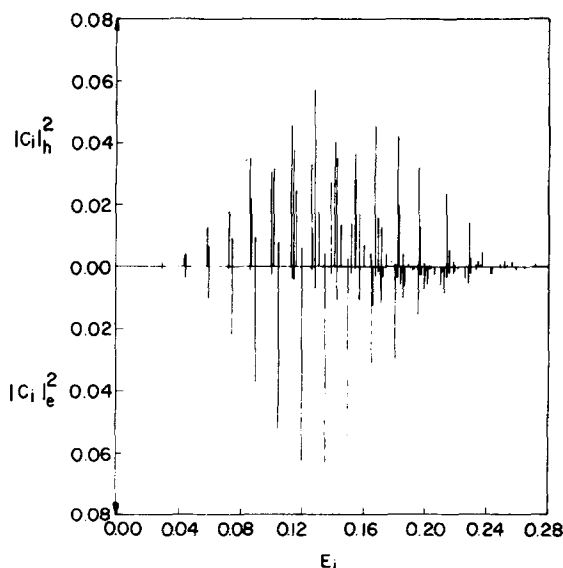


FIG. 6. Population of the various energy levels for the unstable wave packet (above the horizontal axis) and the stable one (below that axis). It is clearly seen that different levels are involved (this would be *strictly* true as $\hbar \rightarrow 0$) and that the levels involved for the stable wave packet are approximately equidistant.

We still have to explain why the regular energy levels are almost equidistant, while the irregular ones are not. The reason is that, if the classical motion is integrable, then in the semiclassical limit (that is, when the action variables I_k are much larger than \hbar) the EBK quantization scheme¹⁷⁻¹⁹ gives very reliable results. We write the Hamiltonian as $H(I_1, \dots, I_n)$ and take $I_k = (m_k + \alpha_k)\hbar$, where the m_k are integers and the α_k are constants. The energy levels are given by²⁰⁻²²

$$E_{m_1 \dots m_n} = H(\alpha_1 \hbar, \dots, \alpha_n \hbar) + \hbar \sum m_k \omega_k + \frac{1}{2} \hbar^2 \sum m_k m_l \partial \omega_k / \partial I_l + \dots, \quad (12)$$

where $\omega_k = \partial H / \partial I_k$ are the classical frequencies. If we neglect the terms of order \hbar^2 and higher terms, the energy levels are equidistant, with spacing $\hbar \omega_k$. Any corrections to the equal spacing law are of order \hbar^2 (or higher) and due to anharmonicity (dependence of ω_k on I_j).

This result is very gratifying in view of the correspondence principle, which should hold for large quantum numbers (see, however, the next section). As classical integrable motion is multiply periodic²³ the only way a small wave packet (in the limit $\hbar \rightarrow 0$) can follow the classical trajectory is if the energy levels are arranged in families with $\Delta E = \hbar \sum n_k \omega_k$, where the n_k are integers and ω_k is any of the classical frequencies.

On the other hand, there is no regularity in the arrangement of quantum energy levels for systems which are classically chaotic.²⁴ Although these levels are *not* completely random (their spacing is subject to a kind of "level repulsion")²⁵⁻²⁸ there is no mechanism to prevent the rapid dephasing of the components C_n .

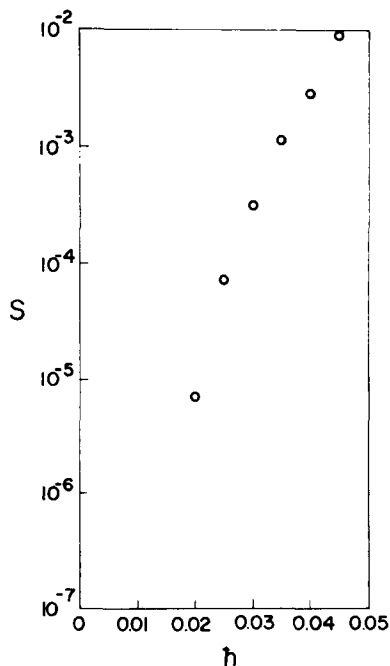


FIG. 7. The overlap S of the two stable wave packets e_1 and e_2 tends to zero as $\hbar \rightarrow 0$.

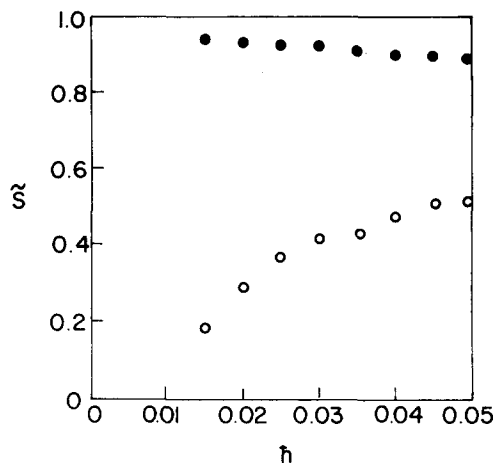


FIG. 8. In contrast to the result of Fig. 7, the "generalized overlap" \tilde{S} of the two stable wave packets (closed circles) tends to 1 as $\hbar \rightarrow 0$. On the other hand, the \tilde{S} of a stable and an unstable wave packet tends to zero (open circles).

Finally, let us note that the transition between regular spectra (equidistant families) and irregular ones cannot be abrupt. In the transition from classically regular to chaotic motion, there appear to be "vague tori" corresponding to approximate constants of motion which are useful for describing the dynamics up to several hundred vibration periods.^{29,30} These remnants of invariant manifolds may provide enough phase space structure to allow some approximate EBK quantization. We thus expect the equidistant level families to *gradually* evolve into "random" spectra, as we proceed from the regular to the irregular region of phase space.

IV. SOME LIMITATIONS OF THE CORRESPONDENCE PRINCIPLE

The "correspondence principle"—the analogy between classical and quantum dynamics—is often used as a guide to discover quantum properties similar to known classical laws. In the foregoing sections, we invoked it several times and obtained results which reasonably fulfilled our expectations. We shall now point out some of its limitations and in particular show that the classical area preserving theorem, which is often considered crucial in discussing chaos, has no quantum analog.

As well known, an important property of classical Hamiltonian trajectories is the existence of Poincaré invariants,^{31,32} the simplest of which can be described as follows. Consider the motion of three neighboring points in phase space. The small triangle which they form has a *constant area*.

The correspondence principle suggests that there should be a similar property in quantum theory. However, one may also argue that Poincaré invariants have *no* quantum analog. Indeed, if we consider two neighboring points \mathbf{r} and $\mathbf{r} + \delta \mathbf{r}$ (here \mathbf{r} denotes collectively all the canonical variables q^k and p_k) we have

$$\delta \mathbf{r}(t) = S(t) \delta \mathbf{r}(0), \quad (13)$$

where the transfer matrix $S(t)$ is symplectic¹⁵ and,

therefore, area preserving. These symplectic matrices form a *noncompact* group.³³ Some of their eigenvalues may be arbitrarily large. On the other hand, the quantum evolution of a dynamical variable A is unitary:

$$A(t) = e^{iHt/\hbar} A(0) e^{-iHt/\hbar} . \quad (14)$$

Unitary matrices form a *compact* group. All their eigenvalues lie on the unit circle.

We may therefore expect the quantum evolution to be qualitatively "milder" than the classical one. For example, if we consider a smooth quantum wave packet (size $\gg \hbar^N$, for N degrees of freedom) and the corresponding classical Gibbs ensemble, their evolution becomes radically different after a finite time.^{28,34} The classical phase space density produces very long and thin filaments with volume $< \hbar^N$. The quantum wave function cannot reproduce these minute details and smoothes them away.

We shall now show explicitly how an "area preserving theorem" is approximately valid for quantum mechanical expectation values, but must ultimately break down for any *nonlinear* system, where wave packets do not spread in a uniform way. We first give an elementary proof of the classical theorem, which we then attempt to mimic in quantum theory. The point at which the analogy fails will become obvious.

For simplicity, let us consider a system with a single degree of freedom, and Hamiltonian

$$H = \frac{1}{2} p^2 + V(q) . \quad (15)$$

The classical equations of motion are

$$\dot{q} = p , \quad (16)$$

$$\dot{p} = -dV(q)/dq . \quad (17)$$

If we consider a neighboring trajectory (denoted by primes) we thus have

$$\frac{d}{dt}(q' - q) = (p' - p) , \quad (18)$$

$$\frac{d}{dt}(p' - p) = -\frac{dV(q')}{dq'} + \frac{dV(q)}{dq} \quad (19)$$

$$= -\frac{d^2V(q)}{dq^2}(q' - q) + O(q' - q)^2 . \quad (20)$$

Introducing a second neighboring trajectory (denoted by double primes) we obtain, to second order in the deviations:

$$\frac{d}{dt}[(q' - q)(p'' - p) - (q'' - q)(p' - p)] = 0 . \quad (21)$$

This proves the classical area preserving theorem, for an infinitesimal triangle in phase space.

In the quantized version, our dynamical variables become *operators* P and Q , and we shall denote their expectation values by p and q :

$$p = \langle P \rangle = (\psi, P\psi) , \quad (22)$$

$$q = \langle Q \rangle = (\psi, Q\psi) . \quad (23)$$

From the Heisenberg equations of motion we obtain

$$\dot{q} = p , \quad (24)$$

$$\dot{p} = -\langle dV(Q)/dQ \rangle . \quad (25)$$

While Eqs. (16) and (24) are formally the same, Eqs. (17) and (25) are not, because, in general,

$$\langle dV(Q)/dQ \rangle \neq dV(q)/dq . \quad (26)$$

As shown below, this is the reason for the failure of the correspondence principle.

Let us evaluate Eq. (25) carefully. We have

$$V(Q) = V(q) + (Q - q) \frac{dV(q)}{dq} + \frac{1}{2}(Q - q)^2 \frac{d^2V(q)}{dq^2} + \dots , \quad (27)$$

whence

$$\frac{dV(Q)}{dQ} = \frac{dV(q)}{dq} + (Q - q) \frac{d^2V(q)}{dq^2} + \frac{1}{2}(Q - q)^2 \frac{d^3V(q)}{dq^3} + \dots . \quad (28)$$

Now, $\langle Q - q \rangle \equiv 0$, and moreover

$$\langle (Q - q)^2 \rangle = (\Delta Q)^2 \quad (29)$$

is the dispersion of Q (the square of the width of the wave packet). We therefore obtain, neglecting $\langle (Q - q)^3 \rangle$ and higher terms:

$$-\left\langle \frac{dV(Q)}{dQ} \right\rangle = -\frac{dV(q)}{dq} - \frac{1}{2} \frac{d^3V(q)}{dq^3} (\Delta Q)^2 . \quad (30)$$

The last term is a kind of "quantum force" with no classical analog.³⁵ It is related to the last term in Eq. (4).

We now pursue the method used in the classical proof and introduce a second state ψ' . We define

$$p' = (\psi', P\psi') , \quad (31)$$

$$q' = (\psi', Q\psi') , \quad (32)$$

and also

$$(\Delta' Q)^2 = (\psi', (Q - q')^2 \psi') . \quad (33)$$

We then have

$$\frac{d}{dt}(q' - q) = (p' - p) , \quad (34)$$

which is formally the same as Eq. (18), and

$$\frac{d}{dt}(p' - p) = -\left(\psi', \frac{dV(Q)}{dQ} \psi'\right) + \left(\psi, \frac{dV(Q)}{dQ} \psi\right) \quad (35)$$

$$\simeq -\left[\frac{d^2V(q)}{dq^2} + \frac{1}{2} \frac{d^4V(q)}{dq^4} (\Delta Q)^2\right](q' - q) - \frac{1}{2} \frac{d^3V(q)}{dq^3} [(\Delta' Q)^2 - (\Delta Q)^2] . \quad (36)$$

It is the last term of Eq. (36) which causes the violation of the area preserving theorem for nonlinear systems.

Indeed, introducing a third state ψ'' , we obtain, instead of Eq. (21),

$$\begin{aligned}
& \frac{d}{dt}[(q' - q)(p'' - p) - (q'' - q)(p' - p)] \\
&= \frac{1}{2} \frac{d^3 V(q)}{dq^3} \{ (q'' - q)[(\Delta' Q)^2 - (\Delta Q)^2] \\
&\quad - (q' - q)[(\Delta'' Q)^2 - (\Delta Q)^2] \}, \\
&\approx \frac{d^3 V(q)}{dq^3} \Delta Q [(q'' - q)(\Delta' Q - \Delta Q) - (q' - q)(\Delta'' Q - \Delta Q)].
\end{aligned} \tag{37}$$

This expression does not vanish in general (except for a linear system, where $d^3 V/dq^3 = 0$). It can be neglected only if the size of the wave packets is much smaller than the distance between the vertices of the (infinitesimal) triangle. This approximation is valid for classical systems, such as in planetary motion, but not for generic quantum systems such as atoms or molecules.

V. SOME OPEN PROBLEMS

The work does not exhaust all possible questions about the evolution of quasiclassical wave packets. Let us briefly mention a few problems worthy of further investigation.

In the regular domain, energy levels are not strictly equidistant. It is their "anharmonic" deviation from equidistance which causes the slow spreading of the wave packet. How is it related to the classical "linear" law^{15,36} of spreading in phase space? Likewise, in the chaotic domain, it would be interesting to retrieve the Lyapunov characteristic numbers (the KSS entropy)³⁷ from properties of the quantum energy spectra, in the semiclassical limit $\hbar \rightarrow 0$.

Moreover, in the quantization of the simplest case—periodic classical motion—the equidistance of quantum energy levels, with $\Delta E = \hbar\omega_{cl}$, is a necessary condition to correctly obtain the semiclassical limit. It is not, however, a sufficient condition. There ought to be also precise *phase* relationships so the wave packet does not disintegrate, to reassemble itself only at the end of each period. We hope to clarify this problem in a future publication.

Note added in proof: The equidistant arrangement of regular levels was empirically found by other authors.^{38,39} It is further discussed in Ref. 40.

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